

Operator

Q/ Define operator, linear operator, commutation and commutator.

→ Operator: An operator is a mathematical entity which operates on a function of a variable to give rise to a new function.

eg.  $\frac{d}{dx}$ ,  $\sin$ ,  $\log$ ,  $\frac{\partial^2}{\partial x^2}$  etc.

Linear operator: An operator  $\hat{A}$  is said to be linear operator if it satisfies the following conditions:

i)  $\hat{A}(c\psi) = c\hat{A}\psi$ .

ii)  $\hat{A}(c_1\psi_1 + c_2\psi_2) = c_1\hat{A}\psi_1 + c_2\hat{A}\psi_2$ .

Commutation and Commutator: Let  $\hat{A}$  and  $\hat{B}$  are two different operators. Now  $\hat{A}\hat{B}\psi$  is meant an operation on  $\psi$  first with  $\hat{B}$  and then with  $\hat{A}$ . Also  $\hat{B}\hat{A}\psi$  is meant an operation on  $\psi$  first with  $\hat{A}$  and then with  $\hat{B}$ .

But  $\hat{A}\hat{B}\psi \neq \hat{B}\hat{A}\psi$ , generally.

e.g. Let  $\hat{A} = x$ ,  $\hat{B} = \frac{d}{dx}$ .

$$\begin{aligned} \therefore \hat{A}\hat{B}\psi &= x \cdot \frac{d}{dx}(\psi) \\ &= x \cdot \frac{d\psi}{dx} \rightarrow (1) \end{aligned}$$

And  $\hat{B}\hat{A}\psi = \frac{d}{dx}(x\psi)$

$$\therefore \hat{B}\hat{A}\psi = x \cdot \frac{d\psi}{dx} + \psi \rightarrow (2)$$

Hence,  $\hat{A}\hat{B}\psi \neq \hat{B}\hat{A}\psi$

$$\Rightarrow (\hat{A}\hat{B} - \hat{B}\hat{A})\psi \neq 0$$

The new operator  $(\hat{A}\hat{B} - \hat{B}\hat{A})$  is the commutator of  $\hat{A}$  and  $\hat{B}$ . In short

$$\hat{A}\hat{B} - \hat{B}\hat{A} = [\hat{A}, \hat{B}]$$

If the commutator of the two operators be zero, we say that the operators commute with each other and if the commutator is not equal to zero then we say that the operator doesn't commute.

Q/ what is Hermitian operator? State the characteristics of Hermitian operator.

→ Hermitian operator: A linear operator  $\hat{F}$  is said to be Hermitian operator if

$$(\psi, \hat{F}\psi) = (\psi, \hat{F}\psi)^*$$
 is satisfied.

$$\text{i.e. } \int \psi^* (\hat{F}\psi) d\tau = \int (\hat{F}\psi)^* \psi d\tau$$

characteristics: (a) The sum of two Hermitian operator is a hermitian operator.

(b) The product of two Hermitian operator is Hermitian if and only if they commute.

(c) Hermitian operator gives real eigenvalues.

Q/ what are observables. How are they express in quantum mechanics.

⇒ (i) Why is an observable in quantum mechanics is represented by Hermitian operator.

→ Observable: A quantity obtained by the process of observation or measurement on a physical system is called an observable. An observable is always a real entity, as it is the result of actual measurement.

(ii) In quantum mechanics observables are represented by Hermitian operators since Hermitian operator gives real eigen values and an observable is always a real entity.



Q/ Prove that if the operator is hermitian then the eigenvalue is real.

→ Let  $\hat{F}$  is Hermitian operator, and.

$$\hat{F}\psi = \lambda\psi \rightarrow (1)$$

where  $\lambda$  and  $\psi$  are the eigen value and eigen function respectively of hermitian operator  $\hat{F}$ .

Since  $\hat{F}$  is hermitian operator,

$$(\psi, \hat{F}\psi) = \langle \psi, \hat{F}\psi \rangle^*$$

$$\Rightarrow \int \psi^* \hat{F}\psi d\tau = \int (\hat{F}\psi)^* \psi d\tau.$$

$$\Rightarrow \int \psi^* \lambda\psi d\tau = \int (\lambda\psi)^* \psi d\tau.$$

$$\Rightarrow (\lambda - \lambda^*) \int \psi^* \psi d\tau = 0$$

$$\Rightarrow \lambda - \lambda^* = 0$$

$$\Rightarrow \lambda = \lambda^*$$

Hence  $\lambda$  must be real quantity. Thus eigenvalues of Hermitian operators are real.

Q/ Prove that if the eigenvalue of an operator is real, it is a Hermitian operator.

$$\Rightarrow \text{Let } \hat{F}\psi = \lambda\psi \rightarrow (1)$$

$$\text{and } \lambda = \lambda^*$$

is the operator  $\hat{F}$  gives real eigen values

Now,

$$(\psi, \hat{F}\psi) = \int \psi^* \hat{F}\psi d\tau$$

$$= \int \psi^* \lambda\psi d\tau$$

$$= \lambda \int \psi^* \psi d\tau \rightarrow (2)$$

$$= \lambda (\psi, \psi) \rightarrow (2)$$

$$\begin{aligned}
 \text{And, } (\psi, f\psi)^* &= \int (f\psi)^* \psi d\tau. \\
 &= \int (f\psi)^* \psi d\tau. \\
 &= \lambda^* \int \psi^* \psi d\tau.
 \end{aligned}$$

$$\Rightarrow (\psi, \hat{F}\psi)^* = \lambda (\psi, \psi) \quad [\because \lambda^* = \lambda] \rightarrow (2)$$

comparing eq<sup>n</sup> (2) and (1) we get-

$$(\psi, \hat{F}\psi) = (\psi, \hat{F}\psi)^*$$

Hence  $\hat{F}$  is a Hermitian operator.

Q. i) Examine whether the operator  $i\frac{\partial}{\partial x}$  is Hermitian or not.

ii) Give example of Hermitian operator.

$$\begin{aligned}
 \rightarrow (\psi, i\frac{\partial}{\partial x} \psi) &= \int_{-\alpha}^{+\alpha} \psi^* i\frac{\partial}{\partial x} \psi dx. \\
 &= i \int_{-\alpha}^{+\alpha} \psi^* \frac{\partial \psi}{\partial x} dx. \\
 &= i \left[ \psi^* \psi \right]_{-\alpha}^{+\alpha} - i \int_{-\alpha}^{+\alpha} \frac{\partial \psi^*}{\partial x} \cdot \psi dx. \\
 &= i \times 0 - i \int_{-\alpha}^{+\alpha} \left( \frac{\partial \psi^*}{\partial x} \right) \psi dx. \\
 &= \int_{-\alpha}^{+\alpha} \left( i \frac{\partial \psi}{\partial x} \right)^* \psi dx.
 \end{aligned}$$

$$\Rightarrow (\psi, i\frac{\partial \psi}{\partial x}) = (\psi, i\frac{\partial \psi}{\partial x})^*$$

Hence,  $i\frac{\partial}{\partial x}$  is hermitian.

e.g:  $i\frac{\partial}{\partial x}$ ,  $\hat{x}$ ,  $\hat{p}$ ,  $\hat{L}$ ,  $\hat{p}(-i\hbar\vec{\nabla})$  are hermitian operator.

i) calculate the commutator for position, and linear momentum operator and hence show that  $(x p_x - p_x x) \psi = i\hbar \psi$ .

(ii) calculate the commutator for time and energy operator.

→ i) [The commutator for two operators  $\hat{A}$  and  $\hat{B}$  written as  $[\hat{A}, \hat{B}]$  is given by,

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

when the operators  $\hat{A}$  and  $\hat{B}$  commute,  $\hat{A}\hat{B} = \hat{B}\hat{A}$ , and when  $\hat{A}$  and  $\hat{B}$  do not commute  $\hat{A}\hat{B} \neq \hat{B}\hat{A}$ .]

$$[x, p_x] = (x p_x - p_x x)$$

$$= \left[ x \left( -i\hbar \frac{\partial}{\partial x} \right) - \left( -i\hbar \frac{\partial}{\partial x} \right) x \right] \rightarrow \textcircled{1}$$

If  $\psi$  is a continuous function of  $x$ , then

$$[x, p_x] = (x p_x - p_x x) \psi$$

$$= -i\hbar \left\{ x \frac{\partial}{\partial x} - \frac{\partial}{\partial x} x \right\} \psi$$

$$= -i\hbar \left\{ x \frac{\partial \psi}{\partial x} - \frac{\partial}{\partial x} (x \psi) \right\}$$

$$= -i\hbar \left\{ x \frac{\partial \psi}{\partial x} - x \frac{\partial \psi}{\partial x} - \psi \right\}$$

$$= +i\hbar \psi \rightarrow \textcircled{2}$$

$$\therefore [x, p_x] = i\hbar \psi$$

$$\Rightarrow (x p_x - p_x x) = i\hbar \psi \quad \text{proved}$$



Note  $[p_x, x] = [x, p_x] = -i\hbar$ .

(iv) Energy operator,  $\hat{E} = i\hbar \frac{\partial}{\partial t}$ .

Time operator,  $\hat{t} = t$ .

$$\begin{aligned} \therefore [\hat{t}, \hat{E}] \psi &= [\hat{t} \hat{E} - \hat{E} \hat{t}] \psi \\ &= [t(i\hbar \frac{\partial}{\partial t}) - i\hbar \frac{\partial}{\partial t} \cdot t] \psi \\ &= i\hbar [t \frac{\partial \psi}{\partial t} - \frac{\partial}{\partial t} (t \psi)] \end{aligned}$$

$$= i\hbar [t \frac{\partial \psi}{\partial t} - t \cdot \frac{\partial \psi}{\partial t} - \psi]$$

$$[\hat{t}, \hat{E}] \psi = -i\hbar \psi, \quad \Rightarrow [\hat{t}, \hat{E}] = -i\hbar.$$

$$\therefore [\hat{E}, \hat{t}] = i\hbar.$$

Prove that

Q/ Any two eigenvectors corresponding to two distinct eigenvalues of a hermitian operator are orthogonal.

→ Proof: Let  $\hat{A}$  is a hermitian operator with eigen functions  $\psi_1$  and  $\psi_2$  corresponding to distinct eigenvalues  $a_1$  and  $a_2$  respectively ( $a_1 \neq a_2$ ).

$$\therefore \hat{A} \psi_1 = a_1 \psi_1 \rightarrow (1)$$

$$\hat{A} \psi_2 = a_2 \psi_2 \rightarrow (2)$$

Now

$$\psi_2^* \hat{A} \psi_1 = \psi_2^* a_1 \psi_1 \rightarrow (3)$$

and

$$\psi_1^* \hat{A} \psi_2 = \psi_1^* a_2 \psi_2 \rightarrow (4)$$

Now taking the conjugate of eq<sup>n</sup> (3).

$$(\psi_2^* \hat{A} \psi_1)^* = (\psi_2^* a_1 \psi_1)^*$$

$$\Rightarrow \psi_1^* \hat{A}^* (\psi_2^*)^* = \psi_1^* a_1^* (\psi_2^*)^*$$

$$\Rightarrow \psi_1^* \hat{A} \psi_2 = a_1^* \psi_1^* \psi_2 \rightarrow (5)$$

Q/ show that,

$$[[A, B], C] + [[B, C], A] + [[C, A], B] = 0$$

Sol<sup>n</sup>:-

$$\begin{aligned} & [[A, B], C] + [[B, C], A] + [[C, A], B] \\ &= [(AB - BA), C] + [(BC - CB), A] + [(CA - AC), B] \\ &= \{ (AB - BA)C - C(AB - BA) \} + \{ (BC - CB)A - A(BC - CB) \} \\ &\quad + \{ (CA - AC)B - B(CA - AC) \} \\ &= \cancel{ABC} - \cancel{BAC} - \cancel{CAB} + \cancel{CBA} + \cancel{BCA} - \cancel{CBA} - \cancel{ACB} + \cancel{ACB} \\ &\quad + \cancel{CAB} - \cancel{ACB} - \cancel{BCA} + \cancel{BCA} - \cancel{CBA} + \cancel{CBA} \\ &= 0. \end{aligned}$$

Q/ what do you mean by expectation value, write down the expectation value of momentum, energy

→ The expectation value is the mathematical expectation for the result of a single measurement or it is the average of the result of a large no. of measurement on independent system.

Let  $\psi(r, t)$  be the wavefunction of a particle normalized to unity. Here  $P(r, t)$  is the position probability density, i.e. the probability of getting the particle at a point  $r$  at time  $t$ .

$$\text{Now, } P(r, t) = \psi^*(r, t) \psi(r, t)$$

Hence the expectation value of the position vector can be mathematically written as,

$$\begin{aligned} \langle r \rangle &= \int r \{ P(r, t) \} dr \\ &= \int \psi^*(r, t) r \psi(r, t) dr. \end{aligned}$$

$$\therefore [\hat{A}^* = A, a_1^\dagger = a]$$

Now, from eq<sup>n</sup> (4) and (5) we get:

$$\psi_1^* a_2 \psi_2 = \psi_1^* a_1 \psi_2$$

$$\Rightarrow \psi_1^* (a_2 - a_1) \psi_2 = 0$$

$$\Rightarrow (a_2 - a_1) \psi_1^* \psi_2 = 0$$

$$\Rightarrow \psi_1^* \psi_2 = 0$$

$\Rightarrow \psi_1$  and  $\psi_2$  are orthogonal. Proved

Q/ If  $\hat{A}$  and  $\hat{B}$  are two operators show that,

$$[\hat{A}, \hat{B}^{-1}] = -\hat{B}^{-1} [\hat{A}, \hat{B}] \hat{B}^{-1}$$

$$\text{Sol:} \quad \text{L.H.S} = [\hat{A}, \hat{B}^{-1}]$$

$$= (\hat{A} \hat{B}^{-1} - \hat{B}^{-1} \hat{A})$$

$$\text{R.H.S} = -\hat{B}^{-1} [\hat{A}, \hat{B}] \hat{B}^{-1}$$

$$= -\hat{B}^{-1} (\hat{A} \hat{B} - \hat{B} \hat{A})$$

$$= -\hat{B}^{-1} (\hat{A} \hat{B} - \hat{B} \hat{A}) \hat{B}^{-1}$$

$$= -\hat{B}^{-1} \hat{A} \hat{B} \hat{B}^{-1} + \hat{B}^{-1} \hat{B} \hat{A} \hat{B}^{-1}$$

$$= -\hat{B}^{-1} \hat{A} + \hat{A} \hat{B}^{-1}$$

$$= \hat{A} \hat{B}^{-1} - \hat{B}^{-1} \hat{A}$$

$$\therefore \text{L.H.S} = \text{R.H.S} \quad \text{Proved}$$



$$\therefore \langle x \rangle = \int \psi^*(x,t) x \psi(x,t) dx$$

$$\langle y \rangle = \int \psi^*(y,t) y \psi(y,t) dy$$

$$\langle z \rangle = \int \psi^*(z,t) z \psi(z,t) dz$$

\* Expectation value of momentum  $\rightarrow$

$$\langle p \rangle = \int \psi^*(r,t) \hat{p} \psi(r,t) dr$$

$$= \int \psi^* (-i\hbar \nabla) \psi dr$$

$$= -i\hbar \int \psi^* \frac{\partial \psi}{\partial x} dx \quad \text{or} \quad -i\hbar \int \psi^* \frac{\partial \psi}{\partial y} dy$$

$$\langle E \rangle = \int \psi^* (i\hbar \frac{\partial}{\partial t}) \psi dr$$

$$\langle H \rangle = \int \psi^* \left( \frac{\hat{p}^2}{2m} + V \right) \psi dr$$

Q. A particle moving in an infinite potential well of width  $L$  in one dimension has the wave function,  $\psi(x) = A \sin \frac{2\pi x}{L}$  for  $-L/2 \leq x \leq L/2$  and  $\psi(x) = 0$  outside.

What is the avg. momentum.

$\rightarrow$  Sol<sup>n</sup>: At first we have to find out the normalized constant.

$$\therefore \int_{-L/2}^{+L/2} \psi^* \psi dx = 1$$

$$\Rightarrow a = \sqrt{\frac{2}{L}}$$

$$\therefore \psi(x) = \sqrt{\frac{2}{L}} \sin \frac{2\pi x}{L}$$

$\therefore$  Expectation/average value of momentum is.

$$\langle p_x \rangle = \int_{-L/2}^{+L/2} \psi^* \hat{p} \psi dx$$

$$\langle \hat{p}_1 \rangle = \left( \sqrt{\frac{2}{L}} \right)^* (-i\hbar) \int_{-L/2}^{+L/2} \sin \frac{2\pi x}{L} \cdot \frac{d}{dx} \left( \sin \frac{2\pi x}{L} \right) dx.$$

$$= -\frac{2}{L} i\hbar \cdot \frac{2\pi}{L} \int_{-L/2}^{+L/2} \sin \frac{2\pi x}{L} \cdot \cos \frac{2\pi x}{L} \cdot dx.$$

$$= -(i\hbar) \frac{2\pi}{L^2} \int_{-L/2}^{+L/2} 2 \sin \frac{2\pi x}{L} \cdot \cos \frac{2\pi x}{L} \cdot dx$$

$$= (-i\hbar) \frac{2\pi}{L^2} \cdot \int_{-L/2}^{+L/2} \sin \frac{4\pi x}{L} \cdot dx.$$

$$= i\hbar \frac{2\pi}{L^2} \left[ \frac{L}{4\pi} \cos \frac{4\pi x}{L} \right]_{-L/2}^{+L/2}$$

$$= 0$$

$$\langle \hat{p}_n \rangle = 0.$$

Question → Find the expectation value  $\langle x \rangle$  of position of a particle in a one dimensional box of length  $L$ .

Sol<sup>n</sup> → for one dimensional box of width  $L$  the wave function is given by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \cdot \sin \frac{n\pi x}{L}.$$

$$\therefore \langle x \rangle = \int_{-\infty}^{\infty} \psi^* \hat{x} \psi \, dx$$

$$\Rightarrow \int_{-L/2}^{+L/2} x |\psi|^2 \, dx.$$

$$= \int_0^L \frac{2}{L} x \sin^2 \frac{n\pi x}{L} \, dx$$

$$= \frac{2}{L} \left[ \int_0^L \frac{x}{2} \cdot 2 \sin^2 \frac{n\pi x}{L} \, dx \right]$$

$$= \frac{1}{L} \left[ \int_0^L x \left( 1 - \cos \frac{2\pi n x}{L} \right) dx \right].$$

$$= \frac{1}{L} \left[ \int_0^L x dx - \int_0^L x \cos \frac{2\pi n x}{L} dx \right]$$

$$= \frac{1}{L} \left[ \frac{x^2}{2} - \frac{x \sin(2\pi n x/L)}{\frac{2\pi n}{L}} - \frac{\cos(2\pi n x/L)}{\frac{4\pi^2 n^2}{L^2}} \right]_0^L$$

Since  $\sin n\pi = 0$ ,  $\cos 2n\pi = 1$ , and  $\cos 0 = 1$ , for all values of  $n$  the expectation value of  $x$  is,

$$\langle x \rangle = \frac{1}{L} \cdot \frac{L^2}{2} = \frac{L}{2}.$$

[ This result means that the average position of the particle is the middle of the box in all  $q.t.$  states. There is no conflict with the fact that  $|\psi|^2 = 0$  at  $L/2$  in the  $n = 2, 4, 6, \dots$  states because  $\langle x \rangle$  is an average not a probability, and it reflects the symmetry of  $|\psi|^2$  about the middle of the box. ]

question: state and prove Ehrenfest theorem.

Ehrenfest theorem  $\Rightarrow$  It states that quantum mechanics yields the same result as classical mechanics for the motion of wave packets associated with moving particle if we use the average or expectation value of dynamical quantities involved.

The proof of the theorem is provided by the equation of motion for the expectation values of position and momentum for a wave packet.

These are:

$$(i) \quad m \cdot \frac{d\langle x \rangle}{dt} = \langle p_x \rangle$$

$$(ii) \quad \frac{d}{dt} \langle p_x \rangle = - \left\langle \frac{dV}{dx} \right\rangle = F_x.$$

$q.t. \rightarrow$  quantum.



(i) Proof  $\rightarrow \frac{d}{dt} \langle x \rangle = \frac{\langle p_x \rangle}{m}$ .

In one dimensional, the expectation value of position co-ordinate  $x$  is given by,

$$\langle x \rangle = \int \psi^* x \psi dx$$

$$\therefore \frac{d}{dt} \langle x \rangle = \frac{d}{dt} \int \psi^* x \psi dx$$

As the operator  $x$  does not depend upon time,

$$\frac{d}{dt} \langle x \rangle = \int \frac{d}{dt} (\psi^* x \psi) dx$$

$$= \int \left( \psi^* x \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} x \psi \right) dx \rightarrow (1)$$

The wave function  $\psi$  satisfies the one dimensional Schrodinger equation,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$\Rightarrow \frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V\psi \rightarrow (2)$$

$$\therefore \frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar} V\psi^* \rightarrow (3)$$

substituting the value of  $\frac{\partial \psi}{\partial t}$  and  $\frac{\partial \psi^*}{\partial t}$  from eq<sup>s</sup> (2) and (3) in eq<sup>n</sup> (1) we get,

$$\frac{d}{dt} \langle x \rangle = \int \left[ \psi^* x \left( \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V\psi \right) + \left( -\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar} V\psi^* \right) x \psi \right] dx$$

$$= \frac{i\hbar}{2m} \int \left( \psi^* x \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2} x \psi \right) dx \rightarrow (4)$$

But  $\frac{\partial^2}{\partial x^2}$  is a Hermitian operator which means

$$\int f^* \frac{\partial^2 g}{\partial x^2} dx = \int \frac{\partial^2 f^*}{\partial x^2} g dx$$

Hence,

$$\int \frac{\partial^2 \psi^*}{\partial x^2} x \psi dx = \int \psi^* \frac{\partial^2 (x \psi)}{\partial x^2} dx.$$

$$= \int \psi^* \frac{\partial}{\partial x} \left( x \frac{\partial \psi}{\partial x} + \psi \right) dx.$$

$$= \int \psi^* \left( x \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial \psi}{\partial x} + \frac{\partial \psi}{\partial x} \right) dx$$

$$= \int \psi^* x \frac{\partial^2 \psi}{\partial x^2} + 2 \int \psi^* \frac{\partial \psi}{\partial x} dx.$$

Substituting in eq<sup>n</sup> (4) we get,

$$\frac{d}{dt} \langle x \rangle = \frac{i\hbar}{2m} \left[ \int \psi^* x \frac{\partial^2 \psi}{\partial x^2} dx - \int \psi^* x \frac{\partial^2 \psi}{\partial x^2} dx - 2 \int \psi^* \frac{\partial \psi}{\partial x} dx \right]$$

$$= -\frac{i\hbar}{m} \int \psi^* \frac{\partial \psi}{\partial x} dx.$$

$$= \frac{1}{m} \int \psi^* \left( -i\hbar \frac{\partial}{\partial x} \right) \psi dx.$$

$$= \frac{1}{m} \int \psi^* p_x \psi dx \quad \left[ \text{because } -i\hbar \frac{\partial}{\partial x} = p_x \right]$$

$$\Rightarrow \frac{d}{dt} \langle x \rangle = \frac{1}{m} \langle p_x \rangle. \quad (\text{Proved})$$

This is the eq<sup>n</sup> of motion for  $\langle x \rangle$  and is the quantum counterpart of classical relation,

Linear momentum = mass  $\times$  velocity.

In three dimension,

$$\frac{d}{dt} \langle \vec{r} \rangle = \frac{1}{m} \langle \vec{P} \rangle.$$

Proved

(i) proof of  $\frac{d}{dt} \langle P_x \rangle = - \langle \frac{dV}{dx} \rangle$ .

(1)

→ the expectation value of x-component of a component of linear momentum  $\langle P_x \rangle$  is given by

$$\langle P_x \rangle = \int \psi^* \left( -i\hbar \frac{\partial}{\partial x} \right) \psi dx$$

$$\therefore \frac{d}{dt} \langle P_x \rangle = \frac{d}{dt} \int \psi^* \left( -i\hbar \frac{\partial}{\partial x} \right) \psi dx$$

$$= -i\hbar \int \left[ \frac{\partial \psi^*}{\partial t} \frac{\partial \psi}{\partial x} + \psi^* \frac{\partial^2 \psi}{\partial x \partial t} \right] dx.$$

$$= \int \left[ -i\hbar \frac{\partial \psi^*}{\partial t} \frac{\partial \psi}{\partial x} - \psi^* i\hbar \frac{\partial^2 \psi}{\partial x \partial t} \right] dx \rightarrow (1)$$

Now, the time dependent schrodinger eq<sup>n</sup> is given by,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \rightarrow (2)$$

$$\Rightarrow i\hbar \frac{\partial^2 \psi}{\partial x \partial t} = -\frac{\hbar^2}{2m} \frac{\partial^3 \psi}{\partial x^3} + \frac{\partial}{\partial x} (V\psi) \rightarrow (3)$$

The complex conjugate of schrodinger eq<sup>n</sup> is,

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + V\psi^* \rightarrow (4)$$

Substituting the value of  $i\hbar \frac{\partial^2 \psi}{\partial x \partial t}$  from eq<sup>n</sup> (3) and  $-i\hbar \frac{\partial^2 \psi^*}{\partial t}$  from eq<sup>n</sup> (4) in eq<sup>n</sup> (1) we have.

$$\frac{d}{dt} \langle P_x \rangle = \int \left[ \left( -\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + V\psi^* \right) \frac{\partial \psi}{\partial x} - \psi^* \left( -\frac{\hbar^2}{2m} \frac{\partial^3 \psi}{\partial x^3} + \frac{\partial (V\psi)}{\partial x} \right) \right] dx.$$

$$= -\frac{\hbar^2}{2m} \int \left[ \frac{\partial^2 \psi^*}{\partial x^2} \frac{\partial \psi}{\partial x} - \psi^* \frac{\partial^3 \psi}{\partial x^3} \right] dx + \int \left[ V\psi^* \frac{\partial \psi}{\partial x} - \psi^* \frac{\partial (V\psi)}{\partial x} \right] dx.$$

$$= -\frac{\hbar^2}{2m} \int \frac{d}{dx} \left( \frac{\partial \psi}{\partial x} \cdot \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right) dx$$

$$+ \int \left[ V\psi^* \frac{\partial \psi}{\partial x} - \psi^* \left( \psi \frac{\partial V}{\partial x} + V \frac{\partial \psi}{\partial x} \right) \right] dx$$



$$= -\frac{\hbar^2}{2m} \int \left[ \frac{d}{dx} \left( \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right) dx \right] + \int -\psi^* \frac{\partial V}{\partial x} \psi dx.$$

Now taking all integrals within the limits  $-\alpha$  to  $+\alpha$ , we have,

$$\frac{d}{dt} \langle p_x \rangle = -\frac{\hbar^2}{2m} \left[ \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right]_{-\alpha}^{+\alpha} + \int_{-\alpha}^{+\alpha} -\psi^* \frac{\partial V}{\partial x} \psi dx.$$

As  $x \rightarrow \alpha$ ,  $\psi$  and  $\frac{\partial \psi}{\partial x} \rightarrow 0$ .  $\therefore$  therefore means.

$$-\frac{\hbar^2}{2m} \left[ \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right]_{-\alpha}^{+\alpha} = 0.$$

$$\therefore \frac{d}{dt} \langle p_x \rangle = - \int_{-\alpha}^{+\alpha} \psi^* \frac{\partial V}{\partial x} \psi dx.$$

$$= \int_{-\alpha}^{+\alpha} \psi^* \left( -\frac{\partial V}{\partial x} \right) \psi dx.$$

$$\therefore \frac{d}{dt} \langle p_x \rangle = - \left\langle \frac{\partial V}{\partial x} \right\rangle, \text{ proved}$$

(The equation of motion for  $\langle p_x \rangle$  is the quantum counterpart of Newton's second law of motion)

question: What do you mean by eigenvalue equation, eigen operator, eigen function and eigen value.

$\rightarrow$  An operator acts on a function to produce a function (same or different). If same function is reproduced the equation is called an eigenvalue equation i.e.

$$\hat{A}\psi = a\psi$$

Here  $\hat{A}$  is called eigen operator,  $\psi$  is called eigen function, and  $a$  is called eigenvalue.

Q/ What is stationary states.

→ If the probability density,  $\rho = |\psi|^2$  is independent of time for a particular state, then the state under consideration is called a stationary state.

$$\text{If } \psi(x, t) = \psi(x) e^{-\frac{iEt}{\hbar}}$$

$$\text{then } \rho = |\psi|^2 = \psi^* \psi$$

$$= |\psi(x)|^2$$

clearly probability density is independent of time therefore  $\psi$  is a stationary state.

Q/ Define: Normalization of  $\psi$ , orthogonal wavefunction, orthonormal wavefunction.

→ Normalization of  $\psi$ : If the probability of finding a particle somewhere in the region is unity, so that,

$$\int |\psi|^2 d\tau = 1,$$

the wave function is called normalized.

[ $d\tau$  represents the small volume w.r.t which the probability of getting the particle is carried out.

orthogonal wavefunction: Two wavefunction  $\psi_m(x)$  and  $\psi_n(x)$  are said to be orthogonal when

$$\int \psi_m(x) \psi_n(x) dx = 0 \quad \text{for}$$

all space

when  $m \neq n$ , where  $m, n = 1, 2, 3, \dots$ . the function  $\psi_m$  and  $\psi_n$  are orthogonal to each other.

orthonormal wavefunction: Functions which hold good for both condition of orthogonality and Normalization are called orthonormal function.



**\*\* Solution of schrodinger eqn :-**

Schrodinger time-dependent eqn for a particle moving along the  $x$ -direction in a potential field  $V$  is given by,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar \frac{\partial \psi}{\partial t} \rightarrow (1)$$

~~Let~~  $\psi(x, t) = u(x)f(t)$ .

using this value in eqn (1) we get.

$$-\frac{\hbar^2}{2m} \cdot f \frac{d^2 u}{dx^2} + Vuf = i\hbar u \cdot \frac{df}{dt} \rightarrow (2)$$

Dividing both side by  $uf$  we get

$$-\frac{\hbar^2}{2m} \cdot \frac{1}{u} \cdot \frac{d^2 u}{dx^2} + V = i\hbar \frac{1}{f} \frac{df}{dt} \rightarrow (3)$$

Here the left hand side of the above eqn is a function of  $x$  and right hand side is a function of  $t$ , so the L.H.S is time independent and R.H.S is the time dependent part of schrodinger equation.

As  $x$  and  $t$  are independent variable each side of eqn (3) must be equal to a constant.

So,

$$-\frac{\hbar^2}{2m} \frac{1}{u} \frac{d^2 u}{dx^2} + V = i\hbar \frac{1}{f} \frac{df}{dt} = E \quad \left[ E = \text{total energy which is const.} \right]$$

Time - dependent part :-

$$i\hbar \frac{1}{f} \frac{df}{dt} = E$$

$$\Rightarrow \frac{df}{f} = \frac{E}{i\hbar} dt$$

$$\Rightarrow \frac{df}{f} = - \frac{iE}{\hbar} dt$$



Integrating the above equation, we get,

$$\begin{aligned}\ln f &= -\frac{iE}{\hbar}t + \ln c \\ \Rightarrow \ln \frac{f}{c} &= -\frac{iE}{\hbar}t \\ \Rightarrow \frac{f}{c} &= e^{-\left(\frac{iE}{\hbar}\right)t} \\ \Rightarrow f(t) &= c e^{-i\left(\frac{E}{\hbar}\right)t} \quad \rightarrow (4)\end{aligned}$$

This is the solution of the time dependent part of the Schrodinger equation.

Time independent part:  $\rightarrow$

$$\begin{aligned}-\frac{\hbar^2}{2m} \frac{1}{u} \cdot \frac{d^2 u}{dx^2} + V &= E \\ \Rightarrow -\frac{\hbar^2}{2m} \frac{d^2 u}{dx^2} + Vu &= Eu \quad \rightarrow (5)\end{aligned}$$

This eq<sup>n</sup> is called one-dimensional steady state Schrodinger equation and its solution  $u(x)$  is known as the time independent wave function or the steady state wave function.

Eq<sup>n</sup> (5) can be expressed as,

$$\frac{d^2 u}{dx^2} + \frac{2m}{\hbar^2} (E - V)u = 0.$$

$\therefore$  The solution of the time-dependent Schrodinger equation is,

$$\psi(x, t) = u(x) f(t) = c u(x) e^{-\frac{iEt}{\hbar}}$$